o-Toluic acid, 2-(1-adamantyl)ethyl ester

Other names: o-toluylic acid, 2-(1-adamantyl)ethyl ester
Inchi: InChI=1S/C20H26O2/c1-14-4-2-3-5-18(14)19(21)22-7-6-20-11-15-8-16(12-20)10-17(9-15
InchiKey: AGTZVGGEDCQSJS-UHFFFAOYSA-N
Formula: C20H26O2
SMILES: Cc1ccccc1C(=O)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	143.33	kJ/mol	Joback Method
hf	-268.73	kJ/mol	Joback Method
hfus	31.07	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.758		Crippen Method
mcvol	243.760	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2416.60		NIST Webbook
tb	785.01	K	Joback Method
tc	1017.93	K	Joback Method
tf	496.22	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.45	J/mol×K	785.01	Joback Method
cpg	802.52	J/mol×K	823.83	Joback Method
cpg	822.82	J/mol×K	862.65	Joback Method
cpg	842.60	J/mol×K	901.47	Joback Method
cpg	862.09	J/mol×K	940.29	Joback Method
cpg	881.54	J/mol×K	979.11	Joback Method
cpg	901.21	J/mol×K	1017.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume